Investigating the Kinetics of Stimulus-Responsive Hydrogels with an Embedded Interface Finite Element Method

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Stimulus-responsive hydrogels (SRHs) are macromolecular polymer networks immersed in a solvent, synthesized to exhibit large volumetric swelling in response to small changes in environmental stimuli. For example, SRHs have been designed to actuate in response to changes in temperature, solvent concentration, pH, and light. The unique properties of these "soft-wet" materials make them appealing for a large range of applications. They have been used for sensors to detect trace contaminants in fuel lines and autonomous control in microfluidic systems, just to name a few. However, a lack of understanding into the relationships between gel composition, kinetics, and mechanical response has hindered designs based on SRHs and delayed the technological transfer from the laboratory to the marketplace.

This presentation will focus on our recent efforts to characterize the unique behavior of SRHs and develop robust finite element models of the same. We have developed continuum-based models for chemically and thermally-induced volume transitions in hydrogels [1,2]. Consistent with experimental observations, the models allow for a sharp interface separating swelled and collapsed phases in SRHs. The models predict characteristic swelling times that are proportional to the square of the characteristic linear dimension of the specimen. Our results have also suggested several synthetic pathways that might be pursued to engineer hydrogels with optimal response times.

The finite element method we have developed to discretize our models relies on an embedded interface representation, wherein the interface geometry is allowed to be independent of the underlying mesh [3,4]. The method enhances the approximation basis in the vicinity of the interface to capture discontinuities in both primary and secondary fields, and is applicable to fully unstructured quad and tet meshes. Interfacial constraints are enforced weakly using a modification of a classical, variationally consistent, interior penalization method. Numerical tests indicate the accuracy of the method to be competitive with widely used finite-difference methods for elliptic interface problems.

References:

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